

# Correlation inequalities for Schrödinger operators

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## Abstract

This paper analyzes Schrödinger operators from viewpoint of correlation inequalities. We construct Griffiths inequalities for the ground state expectations by applying operator-theoretic correlation inequalities. As an example of such an application, we analyze the momentum distribution, i.e., the Fourier transform of the ground state density.

## 1 Introduction

Let us consider the Ising model on  $\Lambda = [-L, L]^d \cap \mathbb{Z}^d$  with  $L \in \mathbb{N}$ . For each spin configuration  $\sigma = \{\sigma_x\}_{x \in \Lambda} \in \Omega = \{-1, +1\}^\Lambda$  on  $\Lambda$ , the energy of the Ising system is

$$H(\sigma) = - \sum_{x, y \in \Lambda} J_{xy} \sigma_x \sigma_y. \quad (1.1)$$

The thermal average is defined by

$$\langle \sigma_A \rangle = \sum_{\sigma \in \Omega} \sigma_A e^{-\beta H(\sigma)} / Z_\beta, \quad Z_\beta = \sum_{\sigma \in \Omega} e^{-\beta H(\sigma)}, \quad (1.2)$$

where  $\sigma_A = \prod_{x \in A} \sigma_x$  for each  $A \subseteq \Lambda$ . In his study of Ising ferromagnets [10, 11, 12], Griffiths discovered the well-known *Griffiths inequalities*. Kelly and Sherman refined the Griffiths inequalities as follows [14]:

- First inequality:

$$\langle \sigma_A \rangle \geq 0, \quad A \subseteq \Lambda; \quad (1.3)$$

- Second inequality:

$$\langle \sigma_A \sigma_B \rangle - \langle \sigma_A \rangle \langle \sigma_B \rangle \geq 0, \quad A, B \subseteq \Lambda. \quad (1.4)$$

These inequalities played an important role in the rigorous study of the Ising model [13]. Accordingly, we can expect that the Griffiths inequalities express the essential idea of correlation in the Ising system. Therefore, it is logical to ask whether similar inequalities hold for other models. An attempt to find a solution to resolve these inequalities can be regarded as an exploration of the model-independent structure of

correlations. Ginibre's work [8] was a first important step toward understanding this model-independent structure. His framework to prove that the Griffiths inequalities still hold for several models [27]. However, we know of a few examples of quantum models that satisfy Griffiths inequalities.

In recent studies, Miyao established the Griffiths inequalities for both Bose and Fermi systems [23]. His theory was constructed from the viewpoint of operator-theoretic correlation inequalities. According to this theory, we can regard reflection positivity in the theory of phase transitions [3, 6, 7] and Lieb's theorem in the Hubbard model [17, 20, 24, 30, 31] as Griffiths inequalities. In this way, the new theory is expected to describe a universal aspect of the notion of correlation.

The Schrödinger operator is undoubtedly one of the most important models in quantum theory. Hence, we can expect that this model will provide a crucial clue, leading to better understanding of the universal aspects of correlation. Conversely, there has been little research on this model from the viewpoint of Griffiths inequalities.<sup>1</sup> The principal aim of the present paper is to analyze the Schrödinger operator in terms of the operator-theoretic correlation inequalities. Through this analysis, we clarify the Griffiths inequalities for ground state expectations. In addition, we study the momentum distribution of the ground state density in terms of the correlation inequalities. Because the forms of the obtained results are consistent with (1.3) and (1.4), we can expect that our analysis actually reveals essence of correlation in Schrödinger operators.

Note that our method can be applied to nonrelativistic quantum field theory [25].

The remainder of this paper is as follows. In Section 2, we display results from the analysis of operator theoretic correlation inequalities.

In Section 3, we construct a general theory of correlation inequalities as operator inequalities associated with self-dual cones. Although many of the results in this section are already proved in previous studies [4, 9, 18, 25, 20, 21, 22, 23, 24], we have specified them here for readers' convenience.

Sections 4-8 are devoted to the analysis of Schrödinger operators in terms of the theory constructed in Section 3.

**Acknowledgments.** This work was partially supported by KAKENHI (20554421) and KAKENHI(16H03942).

## 2 Results

### 2.1 Definitions and assumptions

We will study the Schrödinger operator,

$$H = -\Delta_x - V \tag{2.1}$$

acting in the Hilbert space  $L^2(\mathbb{R}^d; dx)$ . As usual,  $\Delta_x$  is the  $d$ -dimensional Laplacian, and  $V$  is a potential.

To state our results, we need the assumptions **(A)**, **(B)**, and **(C)** below.

Our first assumption concerns the self-adjointness of  $H$ .

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<sup>1</sup> For example, see [1, 16]. In [1], Hydrogen-like atoms in constant magnetic field are studied. In [16], the Born-Oppenheimer energy is investigated.

**(A)** The potential  $V : \mathbb{R}^d \rightarrow \mathbb{R}$  is chosen such that  $H$  is self-adjoint on  $\text{dom}(-\Delta_x)$  and bounded from below.  $\diamond$

**Example 1** If  $V \in L^n(\mathbb{R}^d; dx) + L^\infty(\mathbb{R}^d; dx)$  with  $n = 2$  for  $d \leq 3$ ,  $n > 2$  for  $d = 4$  and  $n = d/2$  for  $d \geq 4$ , then  $V$  satisfies **(A)**, see, e.g., [28, Theorem X. 29].  $\diamond$

**(B)** There exists an approximate sequence  $V_n \neq 0$  for  $V$  such that (i)–(iii) hold:

- (i) Let  $H_n = -\Delta_x - V_n$ .  $H_n$  converges to  $H$  in the strong resolvent sense as  $n \rightarrow \infty$ .<sup>2</sup>
- (ii) For all  $n \in \mathbb{N}$  and a.e.  $p$ , the Fourier transform of  $V_n$ , namely,

$$\hat{V}_n(p) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} dx e^{-ip \cdot x} V_n(x) \quad (2.2)$$

exists and satisfies  $\hat{V}_n \in L^1(\mathbb{R}^d; dp)$ ,  $\hat{V}_n(p) \geq 0$  and  $\hat{V}_n(-p) = \hat{V}_n(p)$  a.e.  $p$ . Moreover, there exists an  $\varepsilon > 0$  such that  $\text{supp} \hat{V}_n \supset B_\varepsilon(0)$ , where  $\text{supp} \hat{V}_n = \{p \in \mathbb{R}^d \mid \hat{V}_n(p) \neq 0\}$  and  $B_\varepsilon(0)$  is the open unit ball centered at the origin of  $\mathbb{R}^d$ .

- (iii)  $\hat{V}_n(p)$  is monotonically increasing in  $n$ , i.e.,  $\hat{V}_n(p) \leq \hat{V}_{n+1}(p)$  a.e.  $p$  for all  $n \in \mathbb{N}$ .  $\diamond$

**Remark 2.1** In concrete applications, it often happens that  $\hat{V}$  does not exist, or that  $\hat{V}$  exists, but  $\hat{V} \notin L^1(\mathbb{R}^d; dp)$ . Even in these cases, we can apply our theory of operator-theoretic correlation inequalities on the basis of assumption **(B)**. This is the principal reason for introducing  $\{V_n\}_{n=1}^\infty$ .  $\diamond$

**Example 2** Let us consider that the Yukawa potential,  $V(x) = \frac{e^{-m|x|}}{|x|}$  with  $m \geq 0$ .

$\hat{V}(p)$  exists and that  $\hat{V}(p) = \frac{2 \cdot 2^{\frac{d}{2}-2}}{p^2 + m^2}$ . Clearly,  $\hat{V}(p) \notin L^1(\mathbb{R}^d; dp)$  for  $d \geq 2$ . In this case, we set

$$V_n(x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{ip \cdot x} \hat{V}_n(p) dp, \quad (2.3)$$

where

$$\hat{V}_n(p) = \begin{cases} \frac{2 \cdot 2^{\frac{d}{2}-2}}{n^{-2} + m^2} & \text{if } |p| \leq \frac{1}{n} \\ \hat{V}(p) & \text{if } \frac{1}{n} < |p| \leq n \\ 0 & \text{if } |p| > n \end{cases} \quad (2.4)$$

Then,  $V_n$  satisfies assumption **(B)**.  $\diamond$

We denote the spectrum of a linear operator  $A$  by  $\sigma(A)$ . The following assumption concerns the least eigenvalue of  $H$ .

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<sup>2</sup> Let  $\{A_n\}_{n=1}^\infty$  be a sequence of self-adjoint operators on  $L^2(\mathbb{R}^d; dx)$ . We say that  $A_n$  converges to  $A$  in the *strong resolvent sense* if  $(A_n - z)^{-1}$  converges to  $(A - z)^{-1}$  in the strong operator topology for all  $z$  with  $\text{Im} z \neq 0$ .

(C) There exists an  $n_0 \in \mathbb{N}$  such that, for all  $n \geq n_0$ ,  $\inf \sigma(H_n)$  is an eigenvalue of  $H_n$ . In addition,  $\inf \sigma(H)$  is an eigenvalue of  $H$ .  $\diamond$

**Definition 2.2** We say that the potential  $V$  is *regular* if it satisfies (A), (B), and (C).  $\diamond$

**Definition 2.3** Let  $A$  be a self-adjoint operator, bounded from below. If  $\inf \sigma(A)$  is an eigenvalue, then the corresponding normalized eigenvectors are called *ground states* of  $A$ .  $\diamond$

The following proposition is a basic input.

**Proposition 2.4** Assume that  $V$  is regular. The ground state of  $H$  (resp.,  $H_n$ ) is unique. Let  $\psi$  (resp.,  $\psi_n$ ) be the unique ground state of  $H$  (resp.,  $H_n$ ).

- (i)  $\psi(x) > 0$  and  $\psi_n(x) > 0$  a.e.  $x$ .
- (ii)  $\hat{\psi}(p) > 0$  and  $\hat{\psi}_n(p) > 0$  a.e.  $p$ .

We prove Proposition 2.4 in Section 4.

We denote by  $\mathcal{B}(\mathfrak{H})$  the set of all bounded linear operators on a Hilbert space  $\mathfrak{H}$ .

**Definition 2.5** Let  $\psi$  (resp.,  $\psi_n$ ) be the unique ground state of  $H$  (resp.,  $H_n$ ). For each  $A \in \mathcal{B}(L^2(\mathbb{R}^d; dx))$ , we define the *ground state expectation*  $\langle A \rangle$  by

$$\langle A \rangle = \langle \psi | A \psi \rangle. \quad (2.5)$$

Similarly, we define  $\langle A \rangle_n = \langle \psi_n | A \psi_n \rangle$ .  $\diamond$

## 2.2 First inequality

Let  $\mathcal{F}$  be the Fourier transform defined by

$$(\mathcal{F}f)(p) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} dx e^{-ip \cdot x} f(x). \quad (2.6)$$

$\mathcal{F}$  is a unitary transformation from  $L^2(\mathbb{R}^d; dx)$  onto  $L^2(\mathbb{R}^d; dp)$ . We often denote  $\mathcal{F}f$  by  $\hat{f}$ .

In this study, we write the operator  $M_f$ , for multiplication by the function  $f$ , simply as  $f$ , if no confusion occurs.

For each  $f \in L^\infty(\mathbb{R}^d; dx)$ , a linear operator  $f(-i\nabla_x)$  is defined by

$$f(-i\nabla_x)\phi = \left( f(p)\hat{\phi} \right)^\vee, \quad \phi \in L^2(\mathbb{R}^d; dx), \quad (2.7)$$

where  $\vee$  is the inverse Fourier transform.

Let

$$\mathfrak{A} = \{ f \in L^\infty(\mathbb{R}^d; dx) \cap L^2(\mathbb{R}^d; dx) \mid \hat{f}(p) \geq 0 \text{ a.e. } p \}. \quad (2.8)$$

The following theorem corresponds to the first Griffiths inequality (1.3).

**Theorem 2.6** Assume that  $V$  is regular.

- (i) For all  $f \in \mathfrak{A}$ ,  $\langle f \rangle \geq 0$ . The equality holds if and only if  $f = 0$ .
- (ii) For all  $f \in \mathfrak{A}$ ,  $\langle f(-i\nabla_x) \rangle \geq 0$ . The equality holds if and only if  $f = 0$ .

We prove Theorem 2.6 in Section 4.

### 2.3 Second inequality

Here, we state some results related to the second Griffiths inequality (1.4). For this purpose, we introduce the following:

$$\mathfrak{A}_e = \{f \in L^\infty(\mathbb{R}^d; dx) \cap L^2(\mathbb{R}^d; dx) \mid \hat{f}(p) \geq 0 \text{ a.e. } p \text{ and } f(-x) = f(x) \text{ a.e. } x\}. \quad (2.9)$$

**Theorem 2.7** *Assume that  $V$  is regular.*

- (i) *For all  $f \in \mathfrak{A}_e$ ,  $\langle f \rangle_n$  is monotonically increasing in  $n$  and converges to  $\langle f \rangle$ .*
- (ii) *For all  $f \in \mathfrak{A}_e$ ,  $\langle f(-i\nabla_x) \rangle_n$  is monotonically decreasing in  $n$  and converges to  $\langle f(-i\nabla_x) \rangle$ .*

We provide a solution of Theorem 2.7 in Section 5.

**Theorem 2.8** *Assume that  $V$  is regular. For all  $f, g \in \mathfrak{A}_e$ , we have the following:*

- (i)  $\langle fg \rangle - \langle f \rangle \langle g \rangle \geq 0$ .
- (ii)  $\langle f(-i\nabla_x)g(-i\nabla_x) \rangle - \langle f(-i\nabla_x) \rangle \langle g(-i\nabla_x) \rangle \geq 0$ .
- (iii)  $\langle f(-i\nabla_x)g \rangle - \langle f(-i\nabla_x) \rangle \langle g \rangle \leq 0$ .

We provide a proof of Theorem 2.8 in Section 6.

**Definition 2.9** Let  $V^{(1)}$  and  $V^{(2)}$  be regular potentials. Let  $\hat{V}_n^{(1)}$  and  $\hat{V}_n^{(2)}$  be the corresponding functions appearing in condition **(B)**. We write  $V^{(1)} \succeq V^{(2)}$ , if there exists an  $n_0 \in \mathbb{N}$  such that for all  $n \geq n_0$ ,  $\hat{V}_n^{(1)}(p) \geq \hat{V}_n^{(2)}(p)$  a.e.  $p$ .  $\diamond$

**Example 3** Let  $W$  be a regular potential. Assume that  $\lambda W$  is regular for all  $\lambda \in I$ , where  $I$  is an open subset of  $(0, \infty)$ . We set  $V^{(1)} = \lambda_1 W$  and  $V^{(2)} = \lambda_2 W$ . If  $\lambda_1, \lambda_2 \in I$  and  $\lambda_1 \geq \lambda_2$ , then  $V^{(1)} \succeq V^{(2)}$ .  $\diamond$

Let  $V^{(1)}$  and  $V^{(2)}$  be regular potentials. We consider Schrödinger operators given by

$$H^{(1)} = -\Delta_x - V^{(1)}, \quad H^{(2)} = -\Delta_x - V^{(2)}. \quad (2.10)$$

Let  $\psi^{(1)}$  (resp.,  $\psi^{(2)}$ ) be the unique ground state of  $H^{(1)}$  (resp.,  $H^{(2)}$ ). We set

$$\langle A \rangle^{(1)} = \langle \psi^{(1)} | A \psi^{(1)} \rangle, \quad \langle A \rangle^{(2)} = \langle \psi^{(2)} | A \psi^{(2)} \rangle. \quad (2.11)$$

In Section 7, we demonstrate the following.

**Theorem 2.10** *Assume that  $V^{(1)}$  and  $V^{(2)}$  are regular.*

- (i) *If  $V^{(1)} \succeq V^{(2)}$ , then  $\langle f \rangle^{(1)} \geq \langle f \rangle^{(2)}$  for all  $f \in \mathfrak{A}_e$ .*
- (ii) *If  $V^{(1)} \succeq V^{(2)}$ , then  $\langle f(-i\nabla_x) \rangle^{(1)} \leq \langle f(-i\nabla_x) \rangle^{(2)}$  for all  $f \in \mathfrak{A}_e$ .*

## 2.4 Applications

Let  $\varrho(x) = |\psi(x)|^2$ . We can apply the above correlation inequalities to investigate properties of  $\varrho(x)$ . Here, we present some examples of applications.

Since  $\varrho \in L^1(\mathbb{R}^d; dx)$ ,  $\hat{\varrho}(p)$  exists for all  $p \in \mathbb{R}^d$  and is continuous in  $p$ .

In Section 8, we prove the following three theorems:

**Theorem 2.11** (i)  $0 < \hat{\varrho}(p)$  for all  $p$ .

(ii)  $\hat{\varrho}(p) \leq \hat{\varrho}(0) = (2\pi)^{-d/2}$  for all  $p$ . There is equality if and only if  $p = 0$ .

(iii)  $(2\pi)^{d/2} \hat{\varrho}(p) \hat{\varrho}(p') \leq \frac{1}{2} \hat{\varrho}(p - p') + \frac{1}{2} \hat{\varrho}(p + p')$  for all  $p, p'$ .

**Theorem 2.12** Assume that  $V$  is regular. Then,  $\hat{\varrho}_n(p)$  is monotonically increasing in  $n$  for all  $p \in \mathbb{R}^d$ .

**Theorem 2.13** Assume that  $V^{(1)}$  and  $V^{(2)}$  are regular, and that  $V^{(1)} \succeq V^{(2)}$ . Let  $\varrho^{(1)}(x) = |\psi^{(1)}(x)|^2$  and  $\varrho^{(2)}(x) = |\psi^{(2)}(x)|^2$ . Then,  $\hat{\varrho}^{(1)}(p) \geq \hat{\varrho}^{(2)}(p)$  for all  $p \in \mathbb{R}^d$ .

**Example 4** Let  $W$  be a regular potential given in Example 3. Let  $\psi_\lambda$  be the unique ground state of  $H_\lambda = -\Delta_x - \lambda W$ , and let  $\varrho_\lambda(x) = |\psi_\lambda(x)|^2$ . Then,  $\hat{\varrho}_\lambda(p)$  is monotonically increasing in  $\lambda \in I$  for all  $p \in \mathbb{R}^d$ .  $\diamond$

## 3 General theory of correlation inequalities

### 3.1 Self-dual cones

Let  $\mathfrak{H}$  be a complex Hilbert space. By a *convex cone*, we understand a closed convex set  $\mathfrak{P} \subset \mathfrak{H}$  such that  $t\mathfrak{P} \subseteq \mathfrak{P}$  for all  $t \geq 0$  and  $\mathfrak{P} \cap (-\mathfrak{P}) = \{0\}$ . In what follows, we always assume that  $\mathfrak{P} \neq \{0\}$ .

**Definition 3.1** The *dual cone* of  $\mathfrak{P}$  is defined by

$$\mathfrak{P}^\dagger = \{\eta \in \mathfrak{H} \mid \langle \eta | \xi \rangle \geq 0 \ \forall \xi \in \mathfrak{P}\}. \quad (3.1)$$

We say that  $\mathfrak{P}$  is *self-dual* if

$$\mathfrak{P} = \mathfrak{P}^\dagger. \quad \diamond \quad (3.2)$$

**Definition 3.2** [4] Let  $\mathfrak{H}$  be a complex Hilbert space. A convex cone  $\mathfrak{P}$  in  $\mathfrak{H}$  is called a *Hilbert cone*, if it satisfies the following:

(i)  $\langle \xi | \eta \rangle \geq 0$  for all  $\xi, \eta \in \mathfrak{P}$ .

(ii) Let  $\mathfrak{H}_\mathbb{R}$  be a real subspace of  $\mathfrak{H}$  generated by  $\mathfrak{P}$ . Then for all  $\xi \in \mathfrak{H}_\mathbb{R}$ , there exist  $\xi_+, \xi_- \in \mathfrak{P}$  such that  $\xi = \xi_+ - \xi_-$  and  $\langle \xi_+ | \xi_- \rangle = 0$ .

(iii)  $\mathfrak{H} = \mathfrak{H}_\mathbb{R} + i\mathfrak{H}_\mathbb{R} = \{\xi + i\eta \mid \xi, \eta \in \mathfrak{H}_\mathbb{R}\}$ .  $\diamond$

**Remark 3.3** Let  $\mathfrak{P}$  be a Hilbert cone in  $\mathfrak{H}$ . For each  $\xi \in \mathfrak{H}$ ,

$$\xi = (\xi_1 - \xi_2) + i(\xi_3 - \xi_4), \quad (3.3)$$

where  $\xi_1, \xi_2, \xi_3$  and  $\xi_4$  satisfy  $\xi_1, \xi_2, \xi_3, \xi_4 \in \mathfrak{P}$ ,  $\langle \xi_1 | \xi_2 \rangle = 0$  and  $\langle \xi_3 | \xi_4 \rangle = 0$ .  $\diamond$

**Theorem 3.4** Let  $\mathfrak{P}$  be a convex cone in  $\mathfrak{H}$ . The following are equivalent:

- (i)  $\mathfrak{P}$  is a self-dual cone.
- (ii)  $\mathfrak{P}$  is a Hilbert cone.

*Proof.* For (i)  $\Rightarrow$  (ii), see, e.g., [2].

Suppose that  $\mathfrak{P}$  is a Hilbert cone. We easily see that  $\mathfrak{P} \subseteq \mathfrak{P}^\dagger$  by Definition 3.2 (i). We will show the inverse. Let  $\xi \in \mathfrak{P}^\dagger$ . By (3.3), we can write  $\xi$  as  $\xi = (\xi_{R,+} - \xi_{R,-}) + i(\xi_{I,+} - \xi_{I,-})$  with  $\xi_{R,\pm}, \xi_{I,\pm} \in \mathfrak{P}$ ,  $\langle \xi_{R,+} | \xi_{R,-} \rangle = 0$  and  $\langle \xi_{I,+} | \xi_{I,-} \rangle = 0$ . Assume that  $\xi_{I,+} \neq 0$ . Then  $\langle \xi | \xi_{I,+} \rangle$  is a complex number, which contradicts with the fact that  $\langle \xi | \eta \rangle \geq 0$  for all  $\eta \in \mathfrak{P}$ . Thus,  $\xi_{I,+} = 0$ . Similarly, we have  $\xi_{I,-} = 0$ . Next, assume that  $\xi_{R,-} \neq 0$ . Because  $\xi_{R,-} \in \mathfrak{P}$ , we have

$$0 \leq \langle \xi | \xi_{R,-} \rangle = -\|\xi_{R,-}\|^2 < 0, \quad (3.4)$$

which is a contradiction. Hence, we conclude that  $\xi = \xi_{R,+} \in \mathfrak{P}$ .  $\square$

**Definition 3.5** • A vector  $\xi$  is said to be *positive w.r.t.  $\mathfrak{P}$*  if  $\xi \in \mathfrak{P}$ . We write this as  $\xi \geq 0$  w.r.t.  $\mathfrak{P}$ .

- A vector  $\eta \in \mathfrak{P}$  is called *strictly positive w.r.t.  $\mathfrak{P}$*  whenever  $\langle \xi | \eta \rangle > 0$  for all  $\xi \in \mathfrak{P} \setminus \{0\}$ . We write this as  $\eta > 0$  w.r.t.  $\mathfrak{P}$ .  $\diamond$

**Example 5** For each  $d \in \mathbb{N}$ , we set

$$L^2(\mathbb{R}^d; du)_+ = \{f \in L^2(\mathbb{R}^d; du) \mid f(u) \geq 0 \text{ a.e. } u\}. \quad (3.5)$$

$L^2(\mathbb{R}^d; du)_+$  is a self-dual cone in  $L^2(\mathbb{R}^d; du)$ .  $f \geq 0$  w.r.t.  $L^2(\mathbb{R}^d; du)_+$  if and only if  $f(u) \geq 0$  a.e.  $u$ . On the other hand,  $f > 0$  w.r.t.  $L^2(\mathbb{R}^d; du)_+$  if and only if  $f(u) > 0$  a.e.  $u$ .  $\diamond$

### 3.2 Operator inequalities associated with self-dual cones

In subsequent sections, we use the following operator inequalities.

**Definition 3.6** We denote by  $\mathcal{B}(\mathfrak{H})$  the set of all bounded linear operators on  $\mathfrak{H}$ . Let  $A, B \in \mathcal{B}(\mathfrak{H})$ . Let  $\mathfrak{P}$  be a self-dual cone in  $\mathfrak{H}$ .

If  $A\mathfrak{P} \subseteq \mathfrak{P}$ ,<sup>3</sup> we then write this as  $A \geq 0$  w.r.t.  $\mathfrak{P}$ .<sup>4</sup> In this case, we say that  $A$  *preserves the positivity w.r.t.  $\mathfrak{P}$* . Suppose that  $A\mathfrak{H}_{\mathbb{R}} \subseteq \mathfrak{H}_{\mathbb{R}}$  and  $B\mathfrak{H}_{\mathbb{R}} \subseteq \mathfrak{H}_{\mathbb{R}}$ . If  $(A - B)\mathfrak{P} \subseteq \mathfrak{P}$ , then we write this as  $A \geq B$  w.r.t.  $\mathfrak{P}$ .  $\diamond$

**Remark 3.7**  $A \geq 0$  w.r.t.  $\mathfrak{P} \iff \langle \xi | A\eta \rangle \geq 0$  for all  $\xi, \eta \in \mathfrak{P}$ .  $\diamond$

<sup>3</sup> For each subset  $\mathfrak{C} \subseteq \mathfrak{H}$ ,  $A\mathfrak{C}$  is defined by  $A\mathfrak{C} = \{Ax \mid x \in \mathfrak{C}\}$ .

<sup>4</sup> This symbol was introduced by Miura [26], see also [15].

The following proposition is fundamental to this paper.

**Proposition 3.8** *Let  $A, B, C, D \in \mathcal{B}(\mathfrak{H})$  and let  $a, b \in \mathbb{R}$ .*

- (i) *If  $A \geq 0, B \geq 0$  w.r.t.  $\mathfrak{P}$  and  $a, b \geq 0$ , then  $aA + bB \geq 0$  w.r.t.  $\mathfrak{P}$ .*
- (ii) *If  $A \geq B \geq 0$  and  $C \geq D \geq 0$  w.r.t.  $\mathfrak{P}$ , then  $AC \geq BD \geq 0$  w.r.t.  $\mathfrak{P}$ .*
- (iii) *If  $A \geq 0$  w.r.t.  $\mathfrak{P}$ , then  $A^* \geq 0$  w.r.t.  $\mathfrak{P}$ .*

*Proof.* (i) is trivial.

(ii) If  $X \geq 0$  and  $Y \geq 0$  w.r.t.  $\mathfrak{P}$ , we have  $XY\mathfrak{P} \subseteq X\mathfrak{P} \subseteq \mathfrak{P}$ . Hence, it holds that  $XY \geq 0$  w.r.t.  $\mathfrak{P}$ . Hence, we have

$$AC - BD = \underbrace{A}_{\geq 0} \underbrace{(C - D)}_{\geq 0} + \underbrace{(A - B)}_{\geq 0} \underbrace{D}_{\geq 0} \geq 0 \quad \text{w.r.t. } \mathfrak{P}.$$

(iii) For each  $\xi, \eta \in \mathfrak{P}$ , we know that

$$\langle \xi | A^* \eta \rangle = \langle \underbrace{A}_{\geq 0} \underbrace{\xi}_{\geq 0} | \underbrace{\eta}_{\geq 0} \rangle \geq 0. \quad (3.6)$$

Thus, by Remark 3.7, we conclude (iii).  $\square$

**Proposition 3.9** *Let  $\{A_n\}_{n=1}^\infty \subseteq \mathcal{B}(\mathfrak{H})$  and let  $A \in \mathcal{B}(\mathfrak{H})$ . Suppose that  $A_n$  converges to  $A$  in the weak operator topology. If  $A_n \geq 0$  w.r.t.  $\mathfrak{P}$  for all  $n \in \mathbb{N}$ , then  $A \geq 0$  w.r.t.  $\mathfrak{P}$ .*

*Proof.* By Remark 3.7,  $\langle \xi | A_n \eta \rangle \geq 0$  for all  $\xi, \eta \in \mathfrak{P}$ . Thus,  $\langle \xi | A \eta \rangle = \lim_{n \rightarrow \infty} \langle \xi | A_n \eta \rangle \geq 0$  for all  $\xi, \eta \in \mathfrak{P}$ . By Remark 3.7 again, we conclude that  $A \geq 0$  w.r.t.  $\mathfrak{P}$ .  $\square$

**Proposition 3.10** *Let  $A$  be a self-adjoint positive operator on  $\mathfrak{H}$ . Assume that  $e^{-\beta A} \geq 0$  w.r.t.  $\mathfrak{P}$  for all  $\beta \geq 0$ . Assume that  $E = \inf \sigma(A)$  is an eigenvalue of  $A$ . Then there exists a nonzero vector  $\xi \in \ker(A - E)$  such that  $\xi \geq 0$  w.r.t.  $\mathfrak{P}$ .*

*Proof.* Let  $\eta \in \mathfrak{H}$ . By Theorem 3.4, we can express  $\eta$  as  $\eta = \eta_R + i\eta_I$  with  $\eta_R, \eta_I \in \mathfrak{H}_\mathbb{R}$ . Now, we define an antilinear involution  $J$  by  $J\eta = \eta_R - i\eta_I$ . Clearly,

$$\eta_R = \frac{1}{2}(\eta + J\eta), \quad \eta_I = \frac{1}{2i}(\eta - J\eta). \quad (3.7)$$

Moreover,  $\mathfrak{H}_\mathbb{R} = \{\eta \in \mathfrak{H} \mid J\eta = \eta\}$ . Because  $e^{-\beta A}\mathfrak{P} \subseteq \mathfrak{P}$ , we see that  $e^{-\beta A}\mathfrak{H}_\mathbb{R} \subseteq \mathfrak{H}_\mathbb{R}$  for all  $\beta \geq 0$ . Hence, for all  $\beta \geq 0$ , we obtain

$$Je^{-\beta A} = e^{-\beta A}J. \quad (3.8)$$

Let  $\xi \in \ker(A - E)$  with  $\xi \neq 0$ .  $\xi$  can be expressed as  $\xi = \xi_R + i\xi_I$  with  $\xi_R, \xi_I \in \mathfrak{H}_\mathbb{R}$ . Because  $\xi \neq 0$ , we have  $\xi_R \neq 0$  or  $\xi_I \neq 0$ . By (3.7) and (3.8), we know that  $\xi_R, \xi_I \in \ker(A - E) \cap \mathfrak{H}_\mathbb{R}$ . Without loss of generality, we may assume that  $\xi_R \neq 0$ . By Definition 3.2 (ii) and Theorem 3.4, we have a unique decomposition  $\xi_R = \xi_{R,+} - \xi_{R,-}$ ,



where  $\xi_{R,\pm} \in \mathfrak{P}$  with  $\langle \xi_{R,+} | \xi_{R,-} \rangle = 0$ . Let  $|\xi_R| = \xi_{R,+} + \xi_{R,-}$ . Because  $\|\xi_R\| = \| |\xi_R| \|$ , we have

$$e^{-\beta E} \|\xi_R\|^2 = \langle \xi_R | e^{-\beta A} \xi_R \rangle \leq \langle |\xi_R| | e^{-\beta A} |\xi_R| \rangle \leq e^{-\beta E} \|\xi_R\|^2. \quad (3.9)$$

Thus,  $|\xi_R| \in \ker(A - E)$ . Clearly,  $|\xi_R| \geq 0$  w.r.t.  $\mathfrak{P}$ .  $\square$

**Theorem 3.11** *Let  $A$  be a self-adjoint positive operator on  $\mathfrak{H}$  and  $B \in \mathcal{B}(\mathfrak{H})$ . Suppose that*

(i)  $e^{-\beta A} \geq 0$  w.r.t.  $\mathfrak{P}$  for all  $\beta \geq 0$ ;

(ii)  $B \geq 0$  w.r.t.  $\mathfrak{P}$ .

*Then we have  $e^{-\beta(A-B)} \geq 0$  w.r.t.  $\mathfrak{P}$  for all  $\beta \geq 0$ .*

*Proof.* By (ii) and Proposition 3.9,

$$e^{\beta B} = \sum_{n \geq 0} \underbrace{\frac{\beta^n}{n!}}_{\geq 0} \underbrace{B^n}_{\geq 0} \geq 0 \quad \text{w.r.t. } \mathfrak{P} \text{ for all } \beta \geq 0. \quad (3.10)$$

Hence,

$$\left( \underbrace{e^{-\beta A/n}}_{\geq 0} \underbrace{e^{\beta B/n}}_{\geq 0} \right)^n \geq 0 \quad \text{w.r.t. } \mathfrak{P} \text{ for all } \beta \geq 0. \quad (3.11)$$

Using the Trotter–Kato product formula and Proposition 3.9, we arrive at the desired assertion.  $\square$

**Theorem 3.12** *Let  $A, B$  be self-adjoint positive operators on  $\mathfrak{H}$ . Assume that  $B = A - C$  with  $C \in \mathcal{B}(\mathfrak{H})$ . Suppose that*

(i)  $e^{-\beta A} \geq 0$  w.r.t.  $\mathfrak{P}$  for all  $\beta \geq 0$ ;

(ii)  $C \geq 0$  w.r.t.  $\mathfrak{P}$ .

*Then we have  $e^{-\beta B} \geq e^{-\beta A}$  w.r.t.  $\mathfrak{P}$  for all  $\beta \geq 0$ .*

*Proof.* By the Duhamel formula, we have the norm-convergent expansion

$$e^{-\beta B} = \sum_{n=0}^{\infty} D_n(\beta), \quad (3.12)$$

$$D_n(\beta) = \int_{S_n(\beta)} e^{-s_1 A} C e^{-s_2 A} C \dots e^{-s_n A} C e^{-(\beta - \sum_{j=1}^n s_j) A}, \quad (3.13)$$

where  $\int_{S_n(\beta)} = \int_0^\beta ds_1 \int_0^{\beta-s_1} ds_2 \dots \int_0^{\beta-\sum_{j=1}^{n-1} s_j} ds_n$  and  $D_0(\beta) = e^{-\beta A}$ . Since  $C \geq 0$  and  $e^{-tA} \geq 0$  w.r.t.  $\mathfrak{P}$  for all  $t \geq 0$ , it holds that

$$\underbrace{C}_{\geq 0} \underbrace{e^{-s_2 A}}_{\geq 0} \dots \underbrace{e^{-s_n A}}_{\geq 0} \underbrace{C}_{\geq 0} \underbrace{e^{-(\beta - \sum_{j=1}^n s_j) A}}_{\geq 0} \geq 0 \quad (3.14)$$

provided that  $s_1 \geq 0, \dots, s_n \geq 0$  and  $\beta - s_1 - \dots - s_n \geq 0$ . Thus, by Proposition 3.9, we obtain  $D_n(\beta) \geq 0$  w.r.t.  $\mathfrak{P}$  for all  $n \geq 0$ . Thus, by (3.12), we have  $e^{-\beta B} \geq D_{n=0}(\beta) = e^{-\beta A}$  w.r.t.  $\mathfrak{P}$  for all  $\beta \geq 0$ .  $\square$

**Definition 3.13** Let  $A \in \mathcal{B}(\mathfrak{H})$ . We write  $A \triangleright 0$  w.r.t.  $\mathfrak{P}$ , if  $A\xi > 0$  w.r.t.  $\mathfrak{P}$  for all  $\xi \in \mathfrak{P} \setminus \{0\}$ . In this case, we say that  $A$  improves the positivity w.r.t.  $\mathfrak{P}$ .  $\diamond$

The following theorem plays an important role.

**Theorem 3.14** (Perron–Frobenius–Faris) *Let  $A$  be a self-adjoint positive operator on  $\mathfrak{H}$ . Suppose that  $0 \leq e^{-tA}$  w.r.t.  $\mathfrak{P}$  for all  $t \geq 0$ , and  $\inf \sigma(A)$  is an eigenvalue. Let  $P_A$  be the orthogonal projection onto the closed subspace spanned by eigenvectors associated with  $\inf \sigma(A)$ . Then, the following are equivalent:*

- (i)  $\dim \operatorname{ran} P_A = 1$  and  $P_A \triangleright 0$  w.r.t.  $\mathfrak{P}$ .
- (ii)  $0 \triangleleft e^{-tA}$  w.r.t.  $\mathfrak{P}$  for all  $t > 0$ .
- (iii) For each  $\xi, \eta \in \mathfrak{P} \setminus \{0\}$ , there exists a  $t > 0$  such that  $\langle \xi | e^{-tA} \eta \rangle > 0$ .

*Proof.* See, e.g., references [4, 18, 29].  $\square$

**Remark 3.15** By (i), there exists a unique  $\xi \in \mathfrak{H}$  such that  $\xi > 0$  w.r.t.  $\mathfrak{P}$  and  $P_A = |\xi\rangle\langle\xi|$ . Of course,  $\xi$  satisfies  $A\xi = \inf \sigma(A)\xi$ .  $\diamond$

**Definition 3.16** Let  $A \in \mathcal{B}(\mathfrak{H})$ . Assume that  $A \geq 0$  w.r.t.  $\mathfrak{P}$ . We say that  $A$  is *ergodic* w.r.t.  $\mathfrak{P}$  if for each  $\xi, \eta \in \mathfrak{P} \setminus \{0\}$ , there exists an  $n \in \{0\} \cup \mathbb{N}$  such that  $\langle \xi | A^n \eta \rangle > 0$ . Note that the number  $n$  could depend on  $\xi$  and  $\eta$ .  $\diamond$

**Theorem 3.17** *Let  $A$  be a self-adjoint positive operator on  $\mathfrak{H}$ , and let  $B \in \mathcal{B}(\mathfrak{H})$ . Set  $H = A - B$ . Suppose the following:*

- (i)  $e^{-\beta A} \geq 0$  w.r.t.  $\mathfrak{P}$  for all  $\beta \geq 0$ .
- (ii)  $B$  is ergodic w.r.t.  $\mathfrak{P}$ .

*Then,  $e^{-\beta H} \triangleright 0$  w.r.t.  $\mathfrak{P}$  for all  $\beta > 0$ .*

*Proof.* We apply Fröhlich’s idea [5] and use the Duhamel expansion:

$$e^{-\beta H} = \sum_{n \geq 0} \mathcal{D}_n(\beta), \quad (3.15)$$

$$\mathcal{D}_n(\beta) = \int_{S_n(\beta)} e^{-s_1 A} B e^{-s_2 A} \dots e^{-s_n A} B e^{-(\beta - \sum_{j=1}^n s_j) A}. \quad (3.16)$$

In a manner similar to that used in the proof of Theorem 3.12, we know that

$$\mathcal{D}_n(\beta) \geq 0, \quad (3.17)$$

$$e^{-s_1 A} B e^{-s_2 A} \dots e^{-s_n A} B e^{-(\beta - \sum_{j=1}^n s_j) A} \geq 0 \quad (3.18)$$

w.r.t.  $\mathfrak{P}$ .

Let  $\xi, \eta \in \mathfrak{P} \setminus \{0\}$ . Since  $e^{-\beta A} \geq 0$  w.r.t.  $\mathfrak{P}$  for all  $\beta \geq 0$ , we have  $e^{-\beta A} \eta \in \mathfrak{P} \setminus \{0\}$ . Let  $\beta > 0$  be fixed arbitrarily. Because  $B$  is ergodic w.r.t.  $\mathfrak{P}$ , there exists an  $n \in \{0\} \cup \mathbb{N}$  such that  $\langle \xi | B^n e^{-\beta A} \eta \rangle > 0$ . Now, let

$$F(s_1, \dots, s_n) = \left\langle \xi \left| e^{-s_1 A} B e^{-s_2 A} \dots e^{-s_n A} B e^{-(\beta - \sum_{j=1}^n s_j) A} \eta \right. \right\rangle. \quad (3.19)$$

By (3.18), it holds that  $F(s_1, \dots, s_n) \geq 0$ . In addition, we have  $F(0, \dots, 0) = \langle \xi | B^n e^{-\beta A} \eta \rangle > 0$ . Because  $F(s_1, \dots, s_n)$  is continuous in  $s_1, \dots, s_n$ , we obtain

$$\langle \xi | \mathcal{D}_n(\beta) \eta \rangle = \int_{S_n(\beta)} F(s_1, \dots, s_n) > 0. \quad (3.20)$$

By (3.15) and (3.17), we see that  $e^{-\beta H} \supseteq \mathcal{D}_n(\beta)$ , which implies

$$\langle \xi | e^{-\beta H} \eta \rangle \geq \langle \xi | \mathcal{D}_n(\beta) \eta \rangle > 0. \quad (3.21)$$

Since  $\xi$  and  $\eta$  are in  $\mathfrak{P} \setminus \{0\}$ , we conclude that  $e^{-\beta H} \eta > 0$  w.r.t.  $\mathfrak{P}$ . Since  $\beta$  is arbitrary, we obtain that  $e^{-\beta H} \triangleright 0$  w.r.t.  $\mathfrak{P}$  for all  $\beta > 0$ .  $\square$

**Lemma 3.18** *Let  $A \in \mathcal{B}(\mathfrak{H})$ . If  $Au = 0$  for all  $u \in \mathfrak{P}$ , then  $A = 0$ .*

*Proof.* By Remark 3.3, each  $u \in \mathfrak{H}$  can be written as  $u = v_1 - v_2 + i(w_1 - w_2)$ , where  $v_1, v_2, w_1, w_2 \in \mathfrak{P}$  such that  $\langle v_1 | v_2 \rangle = 0$  and  $\langle w_1 | w_2 \rangle = 0$ . Thus, the assumption implies that  $Au = 0$  for all  $u \in \mathfrak{H}$ .  $\square$

**Lemma 3.19** *Let  $A \in \mathcal{B}(\mathfrak{H})$  with  $A \neq 0$ . Assume that  $u > 0$  w.r.t.  $\mathfrak{P}$ . If  $A \supseteq 0$  w.r.t.  $\mathfrak{P}$ , then  $Au \neq 0$ .*

*Proof.* Assume that  $Au = 0$ . Then,  $\langle v | Au \rangle = 0$  for all  $v \in \mathfrak{P}$ , implying that  $\langle A^* v | u \rangle = 0$ . Since  $u > 0$  and  $A^* v \geq 0$  w.r.t.  $\mathfrak{P}$ , we conclude that  $A^* v$  must be zero. Because  $v$  is arbitrary,  $A^* = 0$  by Lemma 3.18.  $\square$

**Corollary 3.20** *Let  $A \in \mathcal{B}(\mathfrak{H})$ . Assume that  $u > 0$  w.r.t.  $\mathfrak{P}$  and  $A \supseteq 0$  w.r.t.  $\mathfrak{P}$ . Then,  $\langle u | Au \rangle = 0$  if and only if  $A = 0$ .*

*Proof.* Suppose that  $\langle u | Au \rangle = 0$ . Assume that  $A \neq 0$ . Since  $Au \geq 0$  and  $u > 0$  w.r.t.  $\mathfrak{P}$ ,  $Au$  must be zero. However, this contradicts Lemma 3.19.  $\square$

### 3.3 A canonical cone in $\mathcal{L}^2(\mathfrak{H})$

Let  $\mathfrak{H}$  be a complex Hilbert space. The set of all Hilbert–Schmidt class operators on  $\mathfrak{H}$  is denoted by  $\mathcal{L}^2(\mathfrak{H})$ , i.e.,  $\mathcal{L}^2(\mathfrak{H}) = \{\xi \in \mathcal{B}(\mathfrak{H}) \mid \text{Tr}[\xi^* \xi] < \infty\}$ . Henceforth, we regard  $\mathcal{L}^2(\mathfrak{H})$  as a Hilbert space equipped with the inner product  $\langle \xi | \eta \rangle_{\mathcal{L}^2} = \text{Tr}[\xi^* \eta]$ ,  $\xi, \eta \in \mathcal{L}^2(\mathfrak{H})$ .

**Definition 3.21** For each  $A \in \mathcal{B}(\mathfrak{H})$ , the *left multiplication operator* is defined by

$$\mathcal{L}(A)\xi = A\xi, \quad \xi \in \mathcal{L}^2(\mathfrak{H}). \quad (3.22)$$

Similarly, the *right multiplication operator* is defined by

$$\mathcal{R}(A)\xi = \xi A, \quad \xi \in \mathcal{L}^2(\mathfrak{H}). \quad (3.23)$$

Note that  $\mathcal{L}(A)$  and  $\mathcal{R}(A)$  belong to  $\mathcal{B}(\mathcal{L}^2(\mathfrak{H}))$ , where  $\mathcal{B}(\mathcal{L}^2(\mathfrak{H}))$  is the set of all bounded linear operators in  $\mathcal{L}^2(\mathfrak{H})$ .  $\diamond$

It is not difficult to check that

$$\mathcal{L}(A)\mathcal{L}(B) = \mathcal{L}(AB), \quad \mathcal{R}(A)\mathcal{R}(B) = \mathcal{R}(BA), \quad A, B \in \mathcal{B}(\mathfrak{H}). \quad (3.24)$$

Let  $\vartheta$  be an antiunitary operator on  $\mathfrak{H}$ .<sup>5</sup> Let  $\Phi_\vartheta$  be an isometric isomorphism from  $\mathcal{L}^2(\mathfrak{H})$  onto  $\mathfrak{H} \otimes \mathfrak{H}$  defined by

$$\Phi_\vartheta(|x\rangle\langle y|) = x \otimes \vartheta y \quad \forall x, y \in \mathfrak{H}. \quad (3.25)$$

Then,

$$\mathcal{L}(A) = \Phi_\vartheta^{-1} A \otimes \mathbb{1} \Phi_\vartheta, \quad \mathcal{R}(\vartheta A^* \vartheta) = \Phi_\vartheta^{-1} \mathbb{1} \otimes A \Phi_\vartheta \quad (3.26)$$

for each  $A \in \mathcal{B}(\mathfrak{H})$ . We write these facts simply as

$$\mathfrak{H} \otimes \mathfrak{H} = \mathcal{L}^2(\mathfrak{H}), \quad A \otimes \mathbb{1} = \mathcal{L}(A), \quad \mathbb{1} \otimes A = \mathcal{R}(\vartheta A^* \vartheta), \quad (3.27)$$

if no confusion arises.

The left and right multiplication operators can be extended to unbounded operators by (3.26) as follows. Let  $A$  be a densely defined closed operator on  $\mathfrak{H}$ . The left multiplication operator  $\mathcal{L}(A)$  and the right multiplication operator  $\mathcal{R}(A)$  are defined as  $\mathcal{L}(A) = \Phi_\vartheta^{-1} A \otimes \mathbb{1} \Phi_\vartheta$  and  $\mathcal{R}(A) = \Phi_\vartheta^{-1} \mathbb{1} \otimes \vartheta A^* \vartheta \Phi_\vartheta$ , respectively.

**Remark 3.22** (i) Both  $\mathcal{L}(A)$  and  $\mathcal{R}(A)$  are closed operators on  $\mathcal{L}^2(\mathfrak{H})$ .

(ii) If  $A$  is self-adjoint, then  $\mathcal{L}(A)$  and  $\mathcal{R}(A)$  are self-adjoint.

(iii) We will also use the conventional identification (3.27).  $\diamond$

Recall that a bounded linear operator  $\xi$  on  $\mathfrak{H}$  is said to be *positive* if  $\langle x | \xi x \rangle_{\mathfrak{H}} \geq 0$  for all  $x \in \mathfrak{H}$ . We write this as  $\xi \geq 0$ .

**Definition 3.23** A canonical cone in  $\mathcal{L}^2(\mathfrak{H})$  is given by

$$\mathcal{L}^2(\mathfrak{H})_+ = \left\{ \xi \in \mathcal{L}^2(\mathfrak{H}) \mid \xi \text{ is self-adjoint and } \xi \geq 0 \text{ as an operator on } \mathfrak{H} \right\}. \quad \diamond \quad (3.28)$$

**Theorem 3.24**  $\mathcal{L}^2(\mathfrak{H})_+$  is a self-dual cone in  $\mathcal{L}^2(\mathfrak{H})$ .

*Proof.* We now check the conditions (i)–(iii) in Definition 3.2.

(i) Let  $\xi, \eta \in \mathcal{L}^2(\mathfrak{H})_+$ . Since  $\xi^{1/2} \eta \xi^{1/2} \geq 0$ , we have  $\langle \xi | \eta \rangle_{\mathcal{L}^2} = \text{Tr}[\xi \eta] = \text{Tr}[\xi^{1/2} \eta \xi^{1/2}] \geq 0$ .

(ii) Note that  $\mathcal{L}^2(\mathfrak{H})_{\mathbb{R}} = \{ \xi \in \mathcal{L}^2(\mathfrak{H}) \mid \xi \text{ is self-adjoint} \}$ . Let  $\xi \in \mathcal{L}^2(\mathfrak{H})_{\mathbb{R}}$ . By the spectral theorem, there is a projection valued measure  $\{E(\cdot)\}$  such that  $\xi = \int_{\mathbb{R}} \lambda dE(\lambda)$ . Denote  $\xi_+ = \int_0^\infty \lambda dE(\lambda)$  and  $\xi_- = \int_{-\infty}^0 (-\lambda) dE(\lambda)$ . Clearly, it holds that  $\xi_+ \xi_- = 0$ ,  $\xi_\pm \in \mathcal{L}^2(\mathfrak{H})_+$  and  $\xi = \xi_+ - \xi_-$ . Thus, (ii) is satisfied.

(iii) For each  $\xi \in \mathcal{L}^2(\mathfrak{H})$ , we have  $\xi = \xi_R + i\xi_I$ , where  $\xi_R = (\xi + \xi^*)/2$  and  $\xi_I = (\xi - \xi^*)/2i$ . Trivially,  $\xi_R, \xi_I \in \mathcal{L}^2(\mathfrak{H})_{\mathbb{R}}$ . Hence,  $\mathcal{L}^2(\mathfrak{H})_+$  is a Hilbert cone. By Theorem 3.4, we conclude that  $\mathcal{L}^2(\mathfrak{H})_+$  is a self-dual cone.  $\square$

**Proposition 3.25** Let  $A \in \mathcal{B}(\mathfrak{H})$ . We have  $\mathcal{L}(A^*)\mathcal{R}(A) \supseteq 0$  w.r.t.  $\mathcal{L}^2(\mathfrak{H})_+$ .

*Proof.* For each  $\xi \in \mathcal{L}^2(\mathfrak{H})_+$ , we have  $\mathcal{L}(A^*)\mathcal{R}(A)\xi = A^* \xi A \geq 0$ .  $\square$

**Remark 3.26** As we noted in references [23, 25], Proposition 3.25 is closely related to spin reflection positivity [17]; see also references [4, 9].  $\diamond$

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<sup>5</sup> We say that a bijective map  $\vartheta$  on  $\mathfrak{H}$  is *antiunitary* if  $\langle \vartheta x | \vartheta y \rangle = \overline{\langle x | y \rangle}$  for all  $x, y \in \mathfrak{H}$ .

## 4 Proofs of Proposition 2.4 and Theorem 2.6

### 4.1 Proof of Proposition 2.4

Let  $H_n = -\Delta_x - V_n$  and let  $\hat{H}_n = \mathcal{F}H_n\mathcal{F}^{-1}$ . We have

$$\hat{H}_n = p^2 - V_n(-i\nabla_p), \quad (4.1)$$

where  $p^2$  stands for the multiplication operator. Of course,  $\hat{H}_n$  acts in  $L^2(\mathbb{R}^d; dp)$ .

**Lemma 4.1** *For all  $n \in \mathbb{N}$ , we have the following:*

- (i)  $V_n(-i\nabla_p) \geq 0$  w.r.t.  $L^2(\mathbb{R}^d; dp)_+$ .
- (ii)  $\exp(-\beta\hat{H}_n) \geq 0$  w.r.t.  $L^2(\mathbb{R}^d; dp)_+$  for all  $\beta \geq 0$ .

*Proof.* Let  $\nabla_p = (D_{p_1}, \dots, D_{p_d})$ , where  $D_{p_j}$  is the (generalized) differential operator on  $L^2(\mathbb{R}^d; dp)$ .

(i) Since  $e^{ik \cdot (-i\nabla_p)}$  is a translation, we see that  $e^{ik \cdot (-i\nabla_p)} \geq 0$  w.r.t.  $L^2(\mathbb{R}^d; dp)_+$  for all  $k \in \mathbb{R}^d$ . Thus, by (ii) of **(B)** and the fact  $\mathcal{F}e^{ik \cdot x}\mathcal{F}^{-1} = e^{ik \cdot (-i\nabla_p)}$ , we have

$$V_n(-i\nabla_p) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{e^{ik \cdot (-i\nabla_p)}}_{\geq 0} \underbrace{\hat{V}_n(p)}_{\geq 0} dp \geq 0 \quad \text{w.r.t. } L^2(\mathbb{R}^d; dp)_+. \quad (4.2)$$

(ii) We know that the multiplication operator  $e^{-\beta p^2}$  satisfies  $e^{-\beta p^2} \geq 0$  w.r.t.  $L^2(\mathbb{R}^d; dp)_+$ . Thus, applying Theorem 3.11, we conclude (ii).  $\square$

Before we proceed, we take note of the following fact.

**Lemma 4.2** *Let  $\mathbb{B}^d$  be the Borel algebra on  $\mathbb{R}^d$ . Let  $B_1, B_2 \in \mathbb{B}^d$  with  $|B_1| > 0$  and  $|B_2| > 0$ , where  $|\cdot|$  is the Lebesgue measure. We set*

$$\mathcal{S}_\varepsilon^{(\ell)} = \left\{ (p, p_1, \dots, p_\ell) \in \mathbb{R}^{d \times (\ell+1)} \mid p \in B_2, p + p_1 + \dots + p_\ell \in B_1, p_1, \dots, p_\ell \in B_\varepsilon(0) \right\}. \quad (4.3)$$

*Then, for each  $\varepsilon > 0$ , there exists an  $\ell \in \mathbb{N}_0 := \{0\} \cup \mathbb{N}$  such that  $|\mathcal{S}_\varepsilon^{(\ell)}| > 0$ .*

*Proof.* Without loss of generality, we may assume that  $B_1$  and  $B_2$  are connected sets. For each  $p_1, \dots, p_\ell \in \mathbb{R}^d$ , we set

$$\mathcal{S}_\varepsilon^{(\ell)}(p_1, \dots, p_\ell) = \left\{ p \in \mathbb{R}^d \mid p \in B_2, p + p_1 + \dots + p_\ell \in B_1 \right\}. \quad (4.4)$$

Note that  $\mathcal{S}_\varepsilon^{(\ell)}(p_1, \dots, p_\ell)$  could be empty. For each  $\varepsilon > 0$ , there exist an  $\ell \in \mathbb{N}_0$  and  $p_1, \dots, p_\ell \in B_\varepsilon(0)$  such that  $|B_2 \cap (B_1 - p_1 - \dots - p_\ell)| > 0$ , where  $B_1 - p_1 - \dots - p_\ell = \{p - p_1 - \dots - p_\ell \mid p \in B_1\}$ . Thus, for these  $\ell \in \mathbb{N}_0$  and  $p_1, \dots, p_\ell \in B_\varepsilon(0)$ ,  $|\mathcal{S}_\varepsilon^{(\ell)}(p_1, \dots, p_\ell)| > 0$ . Because  $|\mathcal{S}_\varepsilon^{(\ell)}(p_1, \dots, p_\ell)|$  is continuous in  $p_1, \dots, p_\ell$ , we have

$$|\mathcal{S}_\varepsilon^{(\ell)}| = \int_{(B_\varepsilon(0))^\ell} dp_1 \dots dp_\ell |\mathcal{S}_\varepsilon^{(\ell)}(p_1, \dots, p_\ell)| > 0. \quad (4.5)$$

This completes the proof.  $\square$

**Proposition 4.3** For each  $n \in \mathbb{N}$ ,  $V_n(-i\nabla_p)$  is ergodic w.r.t.  $L^2(\mathbb{R}^d; dp)_+$ .

*Proof.* Recall that, by (ii) of the assumption **(B)**, there exists an  $\varepsilon > 0$  such that  $\text{supp} \hat{V}_n \supset B_\varepsilon(0)$ .

Let  $f_1, f_2 \in L^2(\mathbb{R}^d; dp)_+ \setminus \{0\}$ . Because  $f_1$  and  $f_2$  are non-zero, there exist  $B_1, B_2 \in \mathbb{B}^d$  such that  $|B_1| > 0$ ,  $|B_2| > 0$ , and  $f_1(p) > 0$  on  $B_1$ ,  $f_2(p) > 0$  on  $B_2$ . By Lemma 4.2, there exists an  $\ell \in \mathbb{N}_0$  such that  $|\mathcal{S}_\varepsilon^{(\ell)}| > 0$ . In addition, we have

$$f_2(p) \left( e^{i(p_1 + \dots + p_\ell) \cdot (-i\nabla_p)} f_1 \right)(p) = f_2(p) f_1(p + p_1 + \dots + p_\ell) > 0 \quad (4.6)$$

for all  $p, p_1, \dots, p_\ell \in \mathbb{R}^d$  such that  $(p, p_1, \dots, p_\ell) \in \mathcal{S}_\varepsilon^{(\ell)}$ . Therefore, we obtain

$$\begin{aligned} & \langle f_2 | V_n^\ell(-i\nabla_p) f_1 \rangle \\ &= (2\pi)^{-nd/2} \int_{\mathbb{R}^d} dp \int_{(\mathbb{R}^d)^\times \ell} dp_1 \dots dp_\ell \hat{V}_n(p_1) \dots \hat{V}_n(p_\ell) f_2(p) f_1(p + p_1 + \dots + p_\ell) \\ &\geq (2\pi)^{-nd/2} \int_{\mathcal{S}_\varepsilon^{(\ell)}} dp dp_1 \dots dp_\ell \underbrace{\hat{V}_n(p_1) \dots \hat{V}_n(p_\ell)}_{>0} \underbrace{f_2(p) f_1(p + p_1 + \dots + p_\ell)}_{>0} \\ &> 0. \end{aligned} \quad (4.7)$$

This completes the proof.  $\square$

**Proposition 4.4** We have  $\exp(-\beta \hat{H}) \triangleright 0$  w.r.t.  $L^2(\mathbb{R}^d; dp)_+$  for all  $\beta > 0$ .

*Proof.* By Lemma 4.1 (ii), Proposition 4.3 and Theorem 3.17, we have  $\exp(-\beta \hat{H}_n) \triangleright 0$  w.r.t.  $L^2(\mathbb{R}^d; dp)_+$  for all  $\beta > 0$  and  $n \in \mathbb{N}$ .

For each  $m, n \in \mathbb{N}$  with  $n \geq m$ ,

$$V_n(-i\nabla_p) - V_m(-i\nabla_p) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{e^{ik \cdot (-i\nabla_p)}}_{\geq 0} \underbrace{(\hat{V}_n(k) - \hat{V}_m(k))}_{\geq 0} dk \geq 0 \quad (4.8)$$

w.r.t.  $L^2(\mathbb{R}^d; dp)_+$ . By Theorem 3.12, we obtain that  $\exp(-\beta \hat{H}_n) \supseteq \exp(-\beta \hat{H}_m)$  w.r.t.  $L^2(\mathbb{R}^d; dp)_+$  for all  $\beta \geq 0$ . Taking  $n \rightarrow \infty$ , we conclude that  $\exp(-\beta \hat{H}) \supseteq \exp(-\beta \hat{H}_m)$  w.r.t.  $L^2(\mathbb{R}^d; dp)_+$  for all  $\beta \geq 0$ , where  $\hat{H} = \mathcal{F}H\mathcal{F}^{-1}$ . Since  $\exp(-\beta \hat{H}_m) \triangleright 0$  w.r.t.  $L^2(\mathbb{R}^d; dp)_+$  for all  $\beta > 0$ , we finally arrive at

$$\exp(-\beta \hat{H}) \supseteq \exp(-\beta \hat{H}_m) \triangleright 0 \text{ w.r.t. } L^2(\mathbb{R}^d; dp)_+ \text{ for all } \beta > 0. \quad (4.9)$$

This completes the proof.  $\square$

*Completion of proof of Proposition 2.4*

It is well-known that  $\exp(-\beta H) \triangleright 0$  and  $\exp(-\beta H_n) \triangleright 0$  w.r.t.  $L^2(\mathbb{R}^d; dx)$  for all  $\beta > 0$ , see, e.g., [29, Theorem XIII. 45]. Thus, we conclude the uniqueness of ground states by Theorem 3.14. Simultaneously, we obtain (i).

By Theorem 3.14 and Proposition 4.4, we conclude (ii).  $\square$

## 4.2 Proof of Theorem 2.6

**Lemma 4.5** *Let  $f \in \mathfrak{A}$ .*

- (i)  $\mathcal{F}f\mathcal{F}^{-1} \geq 0$  w.r.t.  $L^2(\mathbb{R}^d; dp)_+$ .
- (ii)  $f(-i\nabla_x) \geq 0$  w.r.t.  $L^2(\mathbb{R}^d; dx)_+$ .

*Proof.* (i) Because  $\mathcal{F}f\mathcal{F}^{-1} = f(-i\nabla_p)$  and  $\mathcal{F}e^{ik \cdot x}\mathcal{F}^{-1} = e^{ik \cdot (-i\nabla_p)} \geq 0$  w.r.t.  $L^2(\mathbb{R}^d; dp)_+$ , we have

$$\mathcal{F}f\mathcal{F}^{-1} = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{\hat{f}(k)}_{\geq 0} \underbrace{e^{ik \cdot (-i\nabla_p)}}_{\geq 0} dk \geq 0 \quad \text{w.r.t. } L^2(\mathbb{R}^d; dp)_+. \quad (4.10)$$

- (ii) Because  $e^{ik \cdot (-i\nabla_x)} \geq 0$  w.r.t.  $L^2(\mathbb{R}^d; dx)_+$ , we have

$$f(-i\nabla_x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{\hat{f}(k)}_{\geq 0} \underbrace{e^{ik \cdot (-i\nabla_x)}}_{\geq 0} dk \geq 0 \quad \text{w.r.t. } L^2(\mathbb{R}^d; dx)_+. \quad (4.11)$$

This completes the proof.  $\square$

*Completion of proof of Theorem 2.6*

- (i) By Lemma 4.5,

$$\langle f \rangle = \underbrace{\langle \hat{\psi} |}_{>0} \underbrace{f(-i\nabla_p)}_{\geq 0} \underbrace{|\hat{\psi} \rangle}_{>0} \geq 0. \quad (4.12)$$

By Corollary 3.20, the equality holds if and only if  $f = 0$ .

We can prove (ii) similarly.  $\square$

## 5 Proof of Theorem 2.7

### 5.1 Extended Hamiltonian

Consider the extended Hamiltonian

$$\mathbb{H}_n = H_n \otimes \mathbb{1} + \mathbb{1} \otimes H_n \quad (5.1)$$

acting in the doubled Hilbert space  $\mathfrak{H}_{\text{ext}} := \mathfrak{H} \otimes \mathfrak{H}$ .

Let us introduce a new coordinate system  $(X_1, X_2)$  by

$$X_1 = \frac{x_2 - x_1}{2}, \quad X_2 = \frac{x_2 + x_1}{2}. \quad (5.2)$$

Trivially,

$$\nabla_{x_1} = -\frac{1}{2}\nabla_{X_1} + \frac{1}{2}\nabla_{X_2}, \quad \nabla_{x_2} = \frac{1}{2}\nabla_{X_1} + \frac{1}{2}\nabla_{X_2}, \quad (5.3)$$

implying

$$-\Delta_{x_1} - \Delta_{x_2} = -\frac{1}{2}\Delta_{X_1} - \frac{1}{2}\Delta_{X_2}. \quad (5.4)$$

We define an antiunitary operator  $\vartheta$  on  $L^2(\mathbb{R}^d; dX)$  by

$$(\vartheta\phi)(X) = \phi(X)^* \quad \text{a.e. } X \quad (5.5)$$

for each  $\phi \in L^2(\mathbb{R}^d; dX)$ . Using  $\vartheta$ , we obtain the following identifications:

$$\begin{aligned} \mathfrak{H}_{\text{ext}} &= L^2(\mathbb{R}^d; dx) \otimes L^2(\mathbb{R}^d; dx) \\ &= L^2(\mathbb{R}^d \times \mathbb{R}^d; dx_1 dx_2) \\ &= L^2(\mathbb{R}^d \times \mathbb{R}^d; dX_1 dX_2) \\ &= L^2(\mathbb{R}^d; dX) \otimes L^2(\mathbb{R}^d; dX) \\ &= \mathcal{L}^2(L^2(\mathbb{R}^d; dX)). \end{aligned} \quad (5.6)$$

In the last equality, we use the identification (3.27) with  $\vartheta$  given by (5.5). Taking the identifications (5.6) into account, we introduce a self-dual cone  $\mathfrak{P}_{\text{ext}}$  in  $\mathfrak{H}_{\text{ext}}$  by

$$\mathfrak{P}_{\text{ext}} = \mathcal{L}^2(L^2(\mathbb{R}^d; dX))_+. \quad (5.7)$$

**Lemma 5.1** *Under the identifications (5.6), we have the following:*

- (i)  $V_n \otimes \mathbb{1} + \mathbb{1} \otimes V_n \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ .
- (ii)  $f \otimes \mathbb{1} \pm \mathbb{1} \otimes f \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$  for each  $f \in \mathfrak{A}_e$ .

*Proof.* We apply Ginibre's idea [8].

(i) By the elementary fact

$$\cos a + \cos b = 2 \cos \frac{a+b}{2} \cos \frac{a-b}{2}, \quad (5.8)$$

we have

$$\begin{aligned} V_n \otimes \mathbb{1} + \mathbb{1} \otimes V_n &= V(x_1) + V(x_2) \\ &= V(X_2 - X_1) + V(X_1 + X_2) \\ &= (2\pi)^{-d/2} \int_{\mathbb{R}^d} \hat{V}_n(p) \left\{ \cos(p \cdot (X_2 - X_1)) + \cos(p \cdot (X_2 + X_1)) \right\} dp \\ &= (2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{2 \hat{V}_n(p)}_{\geq 0} \underbrace{\mathcal{L}[\cos(p \cdot X)] \mathcal{R}[\cos(p \cdot X)]}_{\geq 0} dp \\ &\geq 0 \quad \text{w.r.t. } \mathfrak{P}_{\text{ext}}. \end{aligned} \quad (5.9)$$

(ii) By (5.8) and

$$\cos a - \cos b = 2 \sin \frac{b+a}{2} \sin \frac{b-a}{2}, \quad (5.10)$$

we have

$$f \otimes \mathbb{1} + \mathbb{1} \otimes f = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{2 \hat{f}(p)}_{\geq 0} \underbrace{\mathcal{L}[\cos(p \cdot X)] \mathcal{R}[\cos(p \cdot X)]}_{\geq 0} dp \geq 0, \quad (5.11)$$

$$f \otimes \mathbb{1} - \mathbb{1} \otimes f = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{2 \hat{f}(p)}_{\geq 0} \underbrace{\mathcal{L}[\sin(p \cdot X)] \mathcal{R}[\sin(p \cdot X)]}_{\geq 0} dp \geq 0 \quad (5.12)$$

w.r.t.  $\mathfrak{P}_{\text{ext}}$ .  $\square$



**Theorem 5.2**  $e^{-\beta \mathbb{H}_n} \succeq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$  for all  $\beta \geq 0$ .

*Proof.* We set  $\mathbb{H}_n = \mathbb{H}_0 - \mathbb{V}_n$ , where  $\mathbb{H}_0 = (-\Delta_x) \otimes \mathbb{1} + \mathbb{1} \otimes (-\Delta_x)$  and  $\mathbb{V}_n = V_n \otimes \mathbb{1} + \mathbb{1} \otimes V_n$ . Note that, by Lemma 5.1, we know that  $\mathbb{V}_n \succeq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ . By (5.4) and the identifications (5.6), we have

$$\mathbb{H}_0 = -\frac{\Delta_{X_1}}{2} - \frac{\Delta_{X_2}}{2} = \mathcal{L}\left[-\frac{\Delta_X}{2}\right] + \mathcal{R}\left[-\frac{\Delta_X}{2}\right]. \quad (5.13)$$

Thus, by Proposition 3.25,

$$e^{-\beta \mathbb{H}_0} = \mathcal{L}[e^{\beta \Delta_X/2}] \mathcal{R}[e^{\beta \Delta_X/2}] \succeq 0 \quad (5.14)$$

w.r.t.  $\mathfrak{P}_{\text{ext}}$ . Now, we can apply Theorem 3.11 and conclude the theorem.  $\square$

**Lemma 5.3** Let  $f \in \mathfrak{A}_e$ . Under the identifications (5.6), we have the following:

- (i)  $f(-i\nabla_x) \otimes \mathbb{1} + \mathbb{1} \otimes f(-i\nabla_x) \succeq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ .
- (ii)  $f(-i\nabla_x) \otimes \mathbb{1} - \mathbb{1} \otimes f(-i\nabla_x) \preceq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ .

*Proof.* Note that

$$\vartheta(-i\nabla_X)\vartheta^{-1} = +i\nabla_X. \quad (5.15)$$

(i) By (5.3) and (5.8),

$$\begin{aligned} & f(-i\nabla_x) \otimes \mathbb{1} + \mathbb{1} \otimes f(-i\nabla_x) \\ &= f(-i\nabla_{x_1}) + f(-i\nabla_{x_2}) \\ &= f\left(\frac{i}{2}\nabla_{X_1} - \frac{i}{2}\nabla_{X_2}\right) + f\left(-\frac{i}{2}\nabla_{X_1} - \frac{i}{2}\nabla_{X_2}\right) \\ &= 2(2\pi)^{-d/2} \int_{\mathbb{R}^d} \hat{f}(p) \cos\left(\frac{-ip \cdot \nabla_{X_1}}{2}\right) \cos\left(\frac{-ip \cdot \nabla_{X_2}}{2}\right) dp \\ &= 2(2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{\hat{f}(p)}_{\geq 0} \underbrace{\mathcal{L}\left[\cos\left(\frac{-ip \cdot \nabla_X}{2}\right)\right] \mathcal{R}\left[\cos\left(\frac{-ip \cdot \nabla_X}{2}\right)\right]}_{\geq 0} dp \\ &\succeq 0 \quad \text{w.r.t. } \mathfrak{P}_{\text{ext}}. \end{aligned} \quad (5.16)$$

This proves (i). Similarly, by (5.3) and (5.10),

$$\begin{aligned} & f(-i\nabla_x) \otimes \mathbb{1} - \mathbb{1} \otimes f(-i\nabla_x) = f\left(\frac{i}{2}\nabla_{X_1} - \frac{i}{2}\nabla_{X_2}\right) - f\left(-\frac{i}{2}\nabla_{X_1} - \frac{i}{2}\nabla_{X_2}\right) \\ &= 2(2\pi)^{-d/2} \int_{\mathbb{R}^d} \hat{f}(p) \sin\left(\frac{-ip \cdot \nabla_{X_1}}{2}\right) \sin\left(\frac{-ip \cdot \nabla_{X_2}}{2}\right) dp \\ &= 2(2\pi)^{-d/2} \int_{\mathbb{R}^d} \hat{f}(p) \mathcal{L}\left[\sin\left(\frac{-ip \cdot \nabla_X}{2}\right)\right] \mathcal{R}\left[\underbrace{\vartheta \sin\left(\frac{-ip \cdot \nabla_X}{2}\right) \vartheta^{-1}}_{= -\sin\left(\frac{-ip \cdot \nabla_X}{2}\right) \text{ by (5.15)}}\right] dp \\ &\preceq 0 \quad \text{w.r.t. } \mathfrak{P}_{\text{ext}}. \end{aligned} \quad (5.17)$$

This proves (ii).  $\square$

## 5.2 Duhamel expansion

Let  $\Omega(x) = \pi^{-d/4} \exp(-|x|^2/2) \in L^2(\mathbb{R}^d; dx)$  and let  $Z_{\beta,n} = \|e^{-\beta H_n} \Omega\|^2$ . We introduce a vector  $\phi_{\beta,n} \in L^2(\mathbb{R}^d; dx)$  by

$$\phi_{\beta,n} = \frac{e^{-\beta H_n} \Omega}{\sqrt{Z_{\beta,n}}}. \quad (5.18)$$

**Lemma 5.4**  $\langle A \rangle_n = \lim_{\beta \rightarrow \infty} \langle \phi_{\beta,n} | A \phi_{\beta,n} \rangle$ .

*Proof.* By Proposition 2.4, we have  $\langle \Omega | \psi_n \rangle > 0$ . Hence, we obtain

$$\psi_n = \text{strong} \lim_{\beta \rightarrow \infty} \phi_{\beta,n}. \quad (5.19)$$

This completes the proof.  $\square$

**Lemma 5.5** Under the identifications (5.6), we have  $\Omega \otimes \Omega \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ .

*Proof.* By (5.2) and (5.6),

$$\Omega \otimes \Omega = \pi^{-d/2} \exp \left\{ -\frac{1}{2} (X_1^2 + X_2^2) \right\} = \tilde{\Omega} \otimes \tilde{\Omega} = |\tilde{\Omega}\rangle \langle \tilde{\Omega}|, \quad (5.20)$$

where  $\tilde{\Omega}(X) = \pi^{-d/4} \exp(-|X|^2/2) \in L^2(\mathbb{R}^d; dX)$ . The RHS of (5.20)  $\geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , because the projection  $|\tilde{\Omega}\rangle \langle \tilde{\Omega}|$  is positive as a linear operator on  $L^2(\mathbb{R}^d; dX)$ .  $\square$

**Theorem 5.6** Let  $A \in \mathcal{B}(L^2(\mathbb{R}^d; dx))$ .

- (i) If  $A \otimes \mathbb{1} - \mathbb{1} \otimes A \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , then  $\langle A \rangle_n$  is monotonically increasing in  $n$ .
- (ii) If  $A \otimes \mathbb{1} - \mathbb{1} \otimes A \leq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , then  $\langle A \rangle_n$  is monotonically decreasing in  $n$ .

*Proof.* Suppose that  $n \geq m$ . Note that

$$\langle A \rangle_n - \langle A \rangle_m = \lim_{\beta \rightarrow \infty} \frac{Z_{\beta,m}}{Z_{\beta,n}} \mathcal{J}_\beta, \quad (5.21)$$

where

$$\mathcal{J}_\beta = \frac{\langle e^{-\beta H_n} \Omega | A e^{-\beta H_n} \Omega \rangle}{Z_{\beta,n}} - \frac{\langle e^{-\beta H_m} \Omega | A e^{-\beta H_m} \Omega \rangle}{Z_{\beta,m}} \frac{Z_{\beta,n}}{Z_{\beta,m}}. \quad (5.22)$$

Let  $\delta = V_n - V_m$ . By the Duhamel formula,

$$e^{-\beta H_n} = e^{-\beta(H_m - \delta)} = \sum_{j \geq 0} \int_{\mathcal{T}_j(\beta)} \delta(s_1) \cdots \delta(s_n) e^{-\beta H_m} ds_1 \cdots ds_n, \quad (5.23)$$

where  $\delta(s) = e^{-s H_m} \delta e^{s H_m}$  and  $\mathcal{T}_j(\beta) = \{(s_1, \dots, s_j) | 0 \leq s_1 \leq \cdots \leq s_j \leq \beta\}$ . The RHS of (5.23) converges in the operator norm topology.

For each  $A \in \mathcal{B}(L^2(\mathbb{R}^d; dx))$ , we set

$$\omega(A) = \langle \phi_{\beta,m} | A \phi_{\beta,m} \rangle. \quad (5.24)$$

By (5.22) and (5.23),

$$\mathcal{J}_\beta = \sum_{i,j \geq 0} \int_{\mathcal{T}_i(\beta)} \int_{\mathcal{T}_j(\beta)} \left\{ \omega(X_i(\mathbf{s})AY_j(\mathbf{t})) - \omega(A)\omega(X_i(\mathbf{s})Y_j(\mathbf{t})) \right\} ds_1 \cdots ds_i dt_1 \cdots dt_j, \quad (5.25)$$

where  $X_i(\mathbf{s}) = \delta(s_i)\delta(s_{i-1}) \cdots \delta(s_1)$  and  $Y_j(\mathbf{t}) = \delta(t_1) \cdots \delta(t_{j-1})\delta(t_j)$ . Thus, to prove the theorem, it suffices to prove the following proposition.

**Proposition 5.7** *Let  $A \in \mathcal{B}(L^2(\mathbb{R}^d; dx))$ .*

(i) *If  $A \otimes \mathbb{1} - \mathbb{1} \otimes A \succeq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , then we have*

$$\omega(X_i(\mathbf{s})AY_j(\mathbf{t})) - \omega(X_i(\mathbf{s})Y_j(\mathbf{t}))\omega(A) \geq 0 \quad (5.26)$$

*for all  $\mathbf{s} \in \mathcal{T}_i(\beta)$  and  $\mathbf{t} \in \mathcal{T}_j(\beta)$ .*

(ii) *If  $A \otimes \mathbb{1} - \mathbb{1} \otimes A \preceq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , then we have*

$$\omega(X_i(\mathbf{s})AY_j(\mathbf{t})) - \omega(X_i(\mathbf{s})Y_j(\mathbf{t}))\omega(A) \leq 0 \quad (5.27)$$

*for all  $\mathbf{s} \in \mathcal{T}_i(\beta)$  and  $\mathbf{t} \in \mathcal{T}_j(\beta)$ .*

*Proof.* (i) For each  $B \in \mathcal{B}(L^2(\mathbb{R}^d; dx))$ , we set

$$B_\pm = B \otimes \mathbb{1} \pm \mathbb{1} \otimes B. \quad (5.28)$$

By (5.8),

$$\delta_+ = 2(2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{(\hat{V}_n(p) - \hat{V}_m(p))}_{\geq 0} \underbrace{\mathcal{L}[\cos(p \cdot X)]\mathcal{R}[\cos(p \cdot X)]}_{\geq 0} dp \succeq 0 \quad \text{w.r.t. } \mathfrak{P}_{\text{ext}}. \quad (5.29)$$

Similarly,  $\delta_- \succeq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ . In addition,  $A_- \succeq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$  by the assumption.

We define

$$X_\pm(\mathbf{s}) = \left[ \prod_{\alpha=1}^i \delta(s_\alpha) \right] \otimes \mathbb{1} \pm \mathbb{1} \otimes \left[ \prod_{\alpha=1}^i \delta(s_\alpha) \right], \quad (5.30)$$

where  $\prod_{\alpha=1}^i B_\alpha = B_i B_{i-1} \cdots B_2 B_1$ , an ordered product. Let

$$\delta_\pm[s] = e^{-s\mathbb{H}_m} \delta_\pm e^{s\mathbb{H}_m}. \quad (5.31)$$

Since  $\delta \otimes \mathbb{1} = \frac{1}{2}(\delta_+ + \delta_-)$  and  $\mathbb{1} \otimes \delta = \frac{1}{2}(\delta_+ - \delta_-)$ , we obtain

$$X_\pm(\mathbf{s}) = 2^{-i} \prod_{\alpha=1}^i \left\{ \delta_+[s_\alpha] + \delta_-[s_\alpha] \right\} \pm 2^{-i} \prod_{\alpha=1}^i \left\{ \delta_+[s_\alpha] - \delta_-[s_\alpha] \right\}. \quad (5.32)$$

For each  $\varepsilon = \{\varepsilon_1, \dots, \varepsilon_i\} \in \{+, -\}^i$ , we define

$$\delta_\varepsilon[\mathbf{s}] = \prod_{\alpha=1}^i \delta_{\varepsilon_\alpha}[s_\alpha]. \quad (5.33)$$

In terms of this notation,

$$\prod_{\alpha=1}^i \left\{ \delta_+[s_\alpha] + \delta_-[s_\alpha] \right\} = \sum_{\varepsilon \in \{+, -\}^i} \delta_\varepsilon[\mathbf{s}], \quad (5.34)$$

$$\prod_{\alpha=1}^i \left\{ \delta_+[s_\alpha] - \delta_-[s_\alpha] \right\} = \sum_{\varepsilon \in \{+, -\}^i} \sigma(\varepsilon) \delta_\varepsilon[\mathbf{s}], \quad (5.35)$$

where  $\sigma(\varepsilon) = (\varepsilon_1 1)(\varepsilon_2 1) \cdots (\varepsilon_i 1) = +1$  if the number of  $\varepsilon_\alpha = -$  is even,  $\sigma(\varepsilon) = -1$  if the number of  $\varepsilon_\alpha = -$  is odd. Thus, we have

$$X_+(\mathbf{s}) = 2^{-(i-1)} \sum_{\sigma(\varepsilon)=+1} \delta_\varepsilon[\mathbf{s}], \quad X_-(\mathbf{s}) = 2^{-(i-1)} \sum_{\sigma(\varepsilon)=-1} \delta_\varepsilon[\mathbf{s}]. \quad (5.36)$$

Because, for each  $\mathbf{s} \in \mathcal{T}_i(\beta)$ ,

$$e^{-\beta \mathbb{H}_m} \delta_\varepsilon[\mathbf{s}] = \underbrace{e^{-(\beta-s_i)\mathbb{H}_m}}_{\geq 0} \underbrace{\delta_{\varepsilon_i}}_{\geq 0} \underbrace{e^{-(s_i-s_{i-1})\mathbb{H}_m}}_{\geq 0} \cdots \underbrace{e^{-(s_2-s_1)\mathbb{H}_m}}_{\geq 0} \underbrace{\delta_{\varepsilon_1}}_{\geq 0} \underbrace{e^{-s_1\mathbb{H}_m}}_{\geq 0} \geq 0 \quad (5.37)$$

w.r.t.  $\mathfrak{P}_{\text{ext}}$ , we conclude that  $e^{-\beta \mathbb{H}_m} X_\pm[\mathbf{s}] \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$  by (5.36). Similarly, we can prove that  $Y_\pm[\mathbf{t}] e^{-\beta \mathbb{H}_m} \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ .

Because

$$\underbrace{e^{-\beta \mathbb{H}_m} X_+(\mathbf{s})}_{\geq 0} \underbrace{A_-}_{\geq 0} \underbrace{Y_-(\mathbf{t}) e^{-\beta \mathbb{H}_m}}_{\geq 0} \geq 0 \quad (5.38)$$

w.r.t.  $\mathfrak{P}_{\text{ext}}$ , we have, by Lemma 5.5,

$$\begin{aligned} & \left\langle \phi_{\beta,m} \otimes \phi_{\beta,m} \middle| X_+(\mathbf{s}) A_- Y_-(\mathbf{t}) \phi_{\beta,m} \otimes \phi_{\beta,m} \right\rangle \\ &= Z_{\beta,n}^{-2} \left\langle \underbrace{\Omega \otimes \Omega}_{\geq 0} \middle| \underbrace{e^{-\beta \mathbb{H}_m} X_+(\mathbf{s}) A_- Y_-(\mathbf{t}) e^{-\beta \mathbb{H}_m}}_{\geq 0} \underbrace{\Omega \otimes \Omega}_{\geq 0} \right\rangle \geq 0, \end{aligned} \quad (5.39)$$

implying that

$$\begin{aligned} & \omega(X_i(\mathbf{s}) A Y_j(\mathbf{t})) - \omega(X_i(\mathbf{s}) Y_j(\mathbf{t})) \omega(A) \\ &+ \omega(A Y_j(\mathbf{t})) \omega(X_i(\mathbf{s})) - \omega(Y_j(\mathbf{t})) \omega(X_i(\mathbf{s}) A) \geq 0. \end{aligned} \quad (5.40)$$

On the other hand, we have  $e^{-\beta \mathbb{H}_m} X_-(\mathbf{s}) A_- Y_+(\mathbf{t}) e^{-\beta \mathbb{H}_m} \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , which implies

$$\begin{aligned} & \omega(X_i(\mathbf{s}) A Y_j(\mathbf{t})) - \omega(X_i(\mathbf{s}) Y_j(\mathbf{t})) \omega(A) \\ &- \omega(A Y_j(\mathbf{t})) \omega(X_i(\mathbf{s})) + \omega(Y_j(\mathbf{t})) \omega(X_i(\mathbf{s}) A) \geq 0. \end{aligned} \quad (5.41)$$

Combining (5.40) and (5.41), we obtain the desired result. We can prove (ii) similarly.

□

*Completion of proof of Theorem 2.7*

By Lemma 5.3 and Theorem 5.6, we conclude Theorem 2.7. □

## 6 Proof of Theorem 2.8

We begin with the following proposition.

**Proposition 6.1** *If  $n > m$ , then  $e^{-\beta\mathbb{H}_n} \geq e^{-\beta\mathbb{H}_m} \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$  for all  $\beta \geq 0$ .*

*Proof.* By (5.29), we already know that  $\delta_+ = \mathbb{V}_n - \mathbb{V}_m \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ . Because  $\mathbb{H}_n = \mathbb{H}_m - \delta_+$ , we conclude the assertion by using Theorem 3.12.  $\square$

Let

$$\mathbb{H} = H \otimes \mathbb{1} + \mathbb{1} \otimes H. \quad (6.1)$$

**Theorem 6.2**  *$e^{-\beta\mathbb{H}} \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$  for all  $\beta \geq 0$ .*

*Proof.* By Proposition 6.1, we know that  $e^{-\beta\mathbb{H}_n} \geq e^{-\beta\mathbb{H}_m} \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$  for all  $\beta \geq 0$ , provided that  $n > m$ . Since  $e^{-\beta\mathbb{H}_n}$  strongly converges to  $e^{-\beta\mathbb{H}}$  by the assumption (B), we obtain  $e^{-\beta\mathbb{H}} \geq e^{-\beta\mathbb{H}_m} \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$  for all  $\beta \geq 0$  by Proposition 3.9.  $\square$

**Corollary 6.3** *Let  $\psi$  be the unique ground state of  $H$ . Under the identifications (5.6),  $\psi \otimes \psi \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ .*

*Proof.* Let  $\Psi = \psi \otimes \psi$ . Since the ground state of  $H$  is unique,  $\Psi$  is the unique ground state of  $\mathbb{H}$ . Thus, by Proposition 3.10 and Theorem 6.2, we conclude the assertion.  $\square$

**Theorem 6.4** *Let  $A, B \in \mathcal{B}(L^2(\mathbb{R}^d; dx))$ . Under the identifications (5.6), we have the following:*

- (i) *If  $A \otimes \mathbb{1} - \mathbb{1} \otimes A \geq 0$  and  $B \otimes \mathbb{1} - \mathbb{1} \otimes B \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , then  $\langle AB \rangle - \langle A \rangle \langle B \rangle \geq 0$ .*
- (ii) *If  $A \otimes \mathbb{1} - \mathbb{1} \otimes A \leq 0$  and  $B \otimes \mathbb{1} - \mathbb{1} \otimes B \leq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , then  $\langle AB \rangle - \langle A \rangle \langle B \rangle \geq 0$ .*
- (iii) *If  $A \otimes \mathbb{1} - \mathbb{1} \otimes A \leq 0$  and  $B \otimes \mathbb{1} - \mathbb{1} \otimes B \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , then  $\langle AB \rangle - \langle A \rangle \langle B \rangle \leq 0$ .*

*Proof.* (i) By Corollary 6.3,

$$2(\langle AB \rangle - \langle A \rangle \langle B \rangle) = \left\langle \underbrace{\psi \otimes \psi}_{\geq 0} \left| \underbrace{(A \otimes \mathbb{1} - \mathbb{1} \otimes A)}_{\geq 0} \underbrace{(B \otimes \mathbb{1} - \mathbb{1} \otimes B)}_{\geq 0} \underbrace{\psi \otimes \psi}_{\geq 0} \right. \right\rangle \geq 0. \quad (6.2)$$

Thus, we obtain (i). We can prove (ii) and (iii) similarly.  $\square$

*Completion of proof of Theorem 2.8*

By Lemmas 5.1, 5.3 and Theorem 6.4, we conclude Theorem 2.8.  $\square$

## 7 Proof of Theorem 2.10

Let  $V_n^{(1)}$  (resp.,  $V_n^{(2)}$ ) be an approximate sequence of  $V^{(1)}$  (resp.,  $V^{(2)}$ ) in condition (B). Let

$$H_n^{(1)} = -\Delta_x - V_n^{(1)}, \quad H_n^{(2)} = -\Delta_x - V_n^{(2)}. \quad (7.1)$$

Then,

$$H_n^{(1)} = H_n^{(2)} - W_n, \quad W_n = V_n^{(1)} - V_n^{(2)}. \quad (7.2)$$

As previously, we study the extended Hamiltonian

$$\mathbb{H}_n^{(1)} = H_n^{(1)} \otimes \mathbb{1} + \mathbb{1} \otimes H_n^{(1)}, \quad \mathbb{H}_n^{(2)} = H_n^{(2)} \otimes \mathbb{1} + \mathbb{1} \otimes H_n^{(2)}. \quad (7.3)$$

By (7.2),

$$\mathbb{W}_n = \mathbb{H}_n^{(1)} - \mathbb{H}_n^{(2)}, \quad \mathbb{W}_n = W_n \otimes \mathbb{1} + \mathbb{1} \otimes W_n. \quad (7.4)$$

**Lemma 7.1**  $\mathbb{W}_n \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ .

*Proof.* In a similar manner as in the proof of Lemma 5.1 (i), we see that

$$\mathbb{W}_n = 2(2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{(\hat{V}_n^{(1)}(k) - \hat{V}_n^{(2)}(k))}_{\geq 0} \underbrace{\mathcal{L}[\cos(k \cdot X)] \mathcal{R}[\cos(k \cdot X)]}_{\geq 0} dk \geq 0 \quad (7.5)$$

w.r.t.  $\mathfrak{P}_{\text{ext}}$ .  $\square$

**Theorem 7.2** Let  $A \in \mathcal{B}(L^2(\mathbb{R}^d; dx))$ .

- (i) If  $A \otimes \mathbb{1} - \mathbb{1} \otimes A \geq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , then  $\langle A \rangle^{(1)} \geq \langle A \rangle^{(2)}$ .
- (ii) If  $A \otimes \mathbb{1} - \mathbb{1} \otimes A \leq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , then  $\langle A \rangle^{(1)} \leq \langle A \rangle^{(2)}$ .

*Proof.* The proof of this theorem is similar to that of Theorem 5.6. Hence, we provide only a sketch of the proof. Let  $\psi_n^{(1)}$  (resp.,  $\psi_n^{(2)}$ ) be the unique ground state of  $H_n^{(1)}$  (resp.,  $H_n^{(2)}$ ). For each  $A \in \mathcal{B}(L^2(\mathbb{R}^d; dx))$ , we set

$$\langle A \rangle_n^{(1)} = \langle \psi_n^{(1)} | A \psi_n^{(1)} \rangle, \quad \langle A \rangle_n^{(2)} = \langle \psi_n^{(2)} | A \psi_n^{(2)} \rangle. \quad (7.6)$$

Corresponding to (5.21), we obtain

$$\langle A \rangle_n^{(1)} - \langle A \rangle_n^{(2)} = \lim_{\beta \rightarrow \infty} \frac{Z_\beta^{(2)}}{Z_\beta^{(1)}} \mathcal{J}_\beta, \quad (7.7)$$

where  $Z_\beta^{(j)} = \|e^{-\beta H_n^{(j)}} \Omega\|^2$  ( $j = 1, 2$ ) and

$$\mathcal{J}_\beta = \frac{\langle e^{-\beta H_n^{(1)}} \Omega | A e^{-\beta H_n^{(1)}} \Omega \rangle}{Z_\beta^{(2)}} - \frac{\langle e^{-\beta H_n^{(2)}} \Omega | A e^{-\beta H_n^{(2)}} \Omega \rangle}{Z_\beta^{(2)}} \frac{Z_\beta^{(1)}}{Z_\beta^{(2)}}. \quad (7.8)$$

Since  $\langle A \rangle^{(\alpha)} = \lim_{n \rightarrow \infty} \langle A \rangle_n^{(\alpha)}$  for each  $\alpha = 1, 2$ , it suffices to prove that  $\mathcal{J}_\beta \geq 0$  for all  $\beta > 0$ .

Let  $\phi_n^{(2)} = e^{-\beta H_n^{(2)}} \Omega / \sqrt{Z_\beta^{(2)}}$ . We set

$$\tilde{\omega}(A) = \left\langle \phi_n^{(2)} \left| A \phi_n^{(2)} \right. \right\rangle, \quad A \in \mathcal{B}(L^2(\mathbb{R}^d; dx)). \quad (7.9)$$

By the Duhamel formula, we obtain

$$\mathcal{J}_\beta = \sum_{i,j \geq 0} \int_{\mathcal{T}_i(\beta)} \int_{\mathcal{T}_j(\beta)} \left\{ \tilde{\omega}(\mathcal{X}_i(\mathbf{s}) A \mathcal{Y}_j(\mathbf{t})) - \tilde{\omega}(A) \tilde{\omega}(\mathcal{X}_i(\mathbf{s}) \mathcal{Y}_j(\mathbf{t})) \right\} ds_1 \cdots ds_i dt_1 \cdots dt_j, \quad (7.10)$$

where  $\mathcal{X}_i(\mathbf{s}) = W_n(s_i) W_n(s_{i-1}) \cdots W_n(s_1)$  and  $\mathcal{Y}_j(\mathbf{t}) = W_n(t_1) \cdots W_n(t_{j-1}) W_n(t_j)$ . By Proposition 7.3 below, the RHS of (7.10) is positive.  $\square$

**Proposition 7.3** *Let  $A \in \mathcal{B}(L^2(\mathbb{R}^d; dx))$ .*

(i) *If  $A \otimes \mathbb{1} - \mathbb{1} \otimes A \succeq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , then we have*

$$\tilde{\omega}(\mathcal{X}_i(\mathbf{s}) A \mathcal{Y}_j(\mathbf{t})) - \tilde{\omega}(\mathcal{X}_i(\mathbf{s}) \mathcal{Y}_j(\mathbf{t})) \tilde{\omega}(A) \geq 0 \quad (7.11)$$

*for all  $\mathbf{s} \in \mathcal{T}_i(\beta)$  and  $\mathbf{t} \in \mathcal{T}_j(\beta)$ .*

(ii) *If  $A \otimes \mathbb{1} - \mathbb{1} \otimes A \preceq 0$  w.r.t.  $\mathfrak{P}_{\text{ext}}$ , then we have*

$$\tilde{\omega}(\mathcal{X}_i(\mathbf{s}) A \mathcal{Y}_j(\mathbf{t})) - \tilde{\omega}(\mathcal{X}_i(\mathbf{s}) \mathcal{Y}_j(\mathbf{t})) \tilde{\omega}(A) \leq 0 \quad (7.12)$$

*for all  $\mathbf{s} \in \mathcal{T}_i(\beta)$  and  $\mathbf{t} \in \mathcal{T}_j(\beta)$ .*

*Proof.* We can prove Proposition 7.3 in a manner similar to that in the proof of Proposition 5.7.  $\square$

*Completion of the proof of Theorem 2.10*

By Lemmas 5.1, 5.3 and Theorem 7.2, we conclude Theorem 2.10.  $\square$

## 8 Proofs of Theorems 2.11, 2.12 and 2.13

### 8.1 Proof of Theorem 2.11

(i) By Theorem 2.6 (i),

$$\langle f \rangle = (2\pi)^{-d/2} \int_{\mathbb{R}} dp \hat{f}(p) \langle \psi | e^{ip \cdot x} \psi \rangle = \int_{\mathbb{R}^d} dp \hat{f}(p) \hat{\varrho}(p) > 0 \quad (8.1)$$

for all  $f \in \mathfrak{A} \cap L^1(\mathbb{R}^d; dx)$  with  $f \neq 0$ . Thus, we conclude (i).

(ii) Since  $V(-x) = V(x)$  a.e.  $x$  by the assumption (ii) of **(B)**, we know that  $\psi(-x) = \psi(x)$  a.e.  $x$ , which implies

$$\langle \psi | \sin(p \cdot x) \psi \rangle = 0. \quad (8.2)$$

Using the elementary fact that  $1 - \cos \theta = 2 \left\{ \sin(\theta/2) \right\}^2$ , we have, by (8.2),

$$1 - (2\pi)^{d/2} \hat{\varrho}(p) = \langle \psi | (\mathbb{I} - e^{-ip \cdot x}) \psi \rangle = 2 \left\langle \psi \left| \left\{ \sin \left( \frac{p \cdot x}{2} \right) \right\}^2 \psi \right. \right\rangle. \quad (8.3)$$

Note that the multiplication operator  $\left\{ \sin \left( \frac{p \cdot x}{2} \right) \right\}^2$  satisfies  $\left\{ \sin \left( \frac{p \cdot x}{2} \right) \right\}^2 \geq 0$  w.r.t.  $L^2(\mathbb{R}^d; dx)_+$ , and is nonzero if and only if  $p \neq 0$ . Hence, by Proposition 2.4 (i) and Corollary 3.20, the RHS of (8.3) is strictly positive if and only if  $p \neq 0$ .

(iii) Note that if  $f \in \mathfrak{A}_e$ , then  $f^* \in \mathfrak{A}_e$  as well. Thus, by Theorem 2.8 (i), we have

$$\langle fg \rangle \geq \langle f \rangle \langle g \rangle, \quad \langle fg^* \rangle \geq \langle f \rangle \langle g^* \rangle. \quad (8.4)$$

Since  $\langle g^* \rangle = \langle g \rangle$ ,

$$\langle fg \rangle + \langle fg^* \rangle \geq 2 \langle f \rangle \langle g \rangle. \quad (8.5)$$

Let  $C_0(\mathbb{R}^d)$  be the set of all continuous functions on  $\mathbb{R}^d$  with compact support. Observe that, for all  $f, g \in \mathfrak{A}_e \cap C_0(\mathbb{R}^d)$ ,

$$\langle fg \rangle = (2\pi)^{-d/2} \int_{\mathbb{R}^d \times \mathbb{R}^d} dp dp' \hat{f}(p) \hat{g}(p') \hat{\varrho}(p + p'), \quad (8.6)$$

$$\langle fg^* \rangle = (2\pi)^{-d/2} \int_{\mathbb{R}^d \times \mathbb{R}^d} dp dp' \hat{f}(p) \hat{g}(p') \hat{\varrho}(p - p') \quad (8.7)$$

and

$$\langle f \rangle \langle g \rangle = \int_{\mathbb{R}^d \times \mathbb{R}^d} dp dp' \hat{f}(p) \hat{g}(p') \hat{\varrho}(p) \hat{\varrho}(p'). \quad (8.8)$$

Since  $\hat{\varrho}(p) > 0$ ,  $\hat{f}(p) \geq 0$  and  $\hat{g}(p) \geq 0$  for all  $f, g \in \mathfrak{A}_e \cap C_0(\mathbb{R}^d)$ , we arrive at

$$(2\pi)^{-d/2} \{ \hat{\varrho}(p + p') + \hat{\varrho}(p - p') \} \geq 2 \hat{\varrho}(p) \hat{\varrho}(p'). \quad (8.9)$$

This completes the proof of (iii).  $\square$

## 8.2 Proofs of Theorems 2.12 and 2.13

These theorems follow immediately from Theorems 2.7 and 2.10.  $\square$

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